arXiv:cond-mat/0402146v4 [cond-mat.mtrl-sci] 10 Oct 2005

Boundary conditions for interfaces of electromagnetic (photonic) crystals and generalized Ewald-Oseen extinction principle

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(Dated: February 2, 2008)

The problem of plane-wave diffraction on semi-infinite orthorhombic electromagnetic (photonic) crystals of general kind is considered. Boundary conditions are obtained in the form of infinite system of equations relating amplitudes of incident wave, eigenmodes excited in the crystal and scattered spatial harmonics. Generalized Ewald-Oseen extinction principle is formulated on the base of deduced boundary conditions. The knowledge of properties of infinite crystal's eigenmodes provides option to solve the diffraction problem for the corresponding semi-infinite crystal numerically. In the case when the crystal is formed by small inclusions which can be treated as point dipolar scatterers with fixed direction the problem admits complete rigorous analytical solution. The amplitudes of excited modes and scattered spatial harmonics are expressed in terms of the wave vectors of the infinite crystal by closed-form analytical formulae. The result is applied for study of reflection properties of metamaterial formed by cubic lattice of split-ring resonators.

PACS numbers: 78.20.Ci, 42.70.Qs, 42.25.Fx, 73.20.Mf

I. INTRODUCTION

Electromagnetic crystals are artificial periodical structures operating at the wavelengths comparable with their periods [1–3]. At the optical frequencies such structures are called as photonic crystals. The inherent feature of these materials is the existence of frequency bands where the crystal does not support propagating waves. The band gaps are caused by spatial resonances of the crystal lattice and strongly depend on the direction of propagation. It means that electromagnetic crystals are media with spatial dispersion [4–6]. The material parameters: permittivity and permeability for such materials, if they can be introduced at all, depend on the wave vector as well as on the frequency. Notice, that the homogenization approach is not the most convenient way for the description of electromagnetic crystals even at low frequencies. It often requires introduction of additional boundary conditions in order to describe boundary problems correctly, and this involves related complexities. The photonic and electromagnetic crystals are usually studied with the help of numerical methods [1–3]. Analytical models exist only for a very narrow class of the crystals. Some types of the crystals can be studied analytically under a certain approximation, but the strict analytical solution for a photonic crystal is an exception.

The goal of the present paper is to demonstrate how boundary problems for electromagnetic crystals can be effectively studied using analytical methods. The paper is separated into the two parts. In the first part the boundary conditions for electromagnetic crystals of general kind are deduced in the form of infinite system of equations relating amplitudes of incident wave, excited eigenmodes of the crystal and scattered spatial harmonics. This system can be interpreted as generalization of well-known Ewald-Oseen extinction principle [7–9] which states that the polarization of dielectric is distributed so that it cancels out the incident wave and produces the propagating wave. For the electromagnetic crystals, inherently periodic structures, the generalized Ewald-Oseen principle states that the polarization of dielectric is distributed so that it cancels out the incident wave as well as all spatial harmonics associated with periodicity of the boundary. This principle expressed in the form of infinite system of boundary conditions provides opportunity to solve the boundary problem for semi-infinite crystal of certain kind numerically if the eigenmode problem for corresponding infinite crystal is already solved. In the second part of the paper the proposed approach is applied for the case of electromagnetic crystals formed by small inclusions which can be treated as point dipolar scatterers with fixed direction. In this case the system of boundary conditions admits complete rigorous analytical solution. The amplitudes of excited eigenmodes and scattered spatial harmonics are expressed in terms of wavevectors of eigenmodes using closed-form analytical formulae. These results are unique extension and generalization of known Mahan-Obermair theory [10] for the case then period of the crystal is compared with wavelength. At the end of the paper it is demonstrated how reflection from the semi-infinite cubic lattice of resonant scatterers (split-ring resonators) can be modeled in the regime of strong spatial dispersion observed in such crystals [11].

II. PROOF OF GENERALIZED EWALD-OSEEN EXTINCTION PRINCIPLE

In this section we provide proof of generalized Ewald-Oseen extinction principle for arbitrary semi-infinite electromagnetic crystal with orthorhombic elementary cell. First, let us consider an infinite orthorhombic electromagnetic crystal with geometry schematically presented in Fig. 1 and characterized by three-periodical permittivity distribution:

$$\overline{\overline{\varepsilon}}(\mathbf{r}) = \overline{\overline{\varepsilon}}(\mathbf{r} + \mathbf{a}n + \mathbf{b}s + \mathbf{c}l). \tag{1}$$

In this expression and in the further text the two lines over a quantity designate that the quantity is dyadic (tensor of second rank in three-dimensional space). It means that we consider of the most general kind of electromagnetic crystals formed by dielectrics.

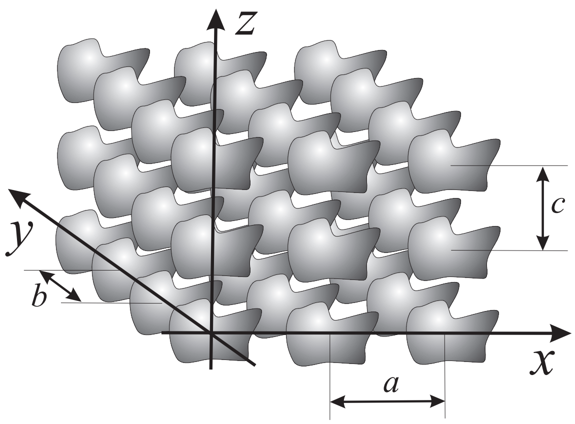

FIG. 1: Geometry of an infinite electromagnetic crystal

In this paper we are using local field approach, an unconventional method for description of fields inside dielectrics. We will operate with local parameters like polarization density $\mathbf{P}$ and local electrical field $\mathbf{E}_{\mathrm{loc.}}$, but not with average electric field $\mathbf{E}$ and displacement $\mathbf{D}$ as usual. The similar approach was used in [9] for rigorous derivation of Ewald-Oseen extinction theorem and in [6]. The dielectric can be treated as a very dense cubic lattice of point scatterers with ceratin local polarizability. In this formulation the dielectric permittivity $\overline{\overline{\varepsilon}}(\mathbf{r})$ has to be replaced (see Figure 2 for illustration) by the local polarizability $\overline{\overline{\alpha}}(\mathbf{r})$ relating the bulk polarization density $\mathbf{P}(\mathbf{r})$ with the local electric field $\mathbf{E}_{\mathrm{loc}}(\mathbf{r})$:

$$\mathbf{P}(\mathbf{r}) = \overline{\overline{\alpha}}(\mathbf{r})\mathbf{E}_{\mathrm{loc}}(\mathbf{r}). \tag{2}$$

The expression for local polarizability in terms of dielectric permittivity has the following form:

$$\overline{\overline{\alpha}}^{-1}(\mathbf{r}) = \left[\overline{\overline{\varepsilon}}(\mathbf{r}) - \varepsilon_0 \overline{\overline{I}}\right]^{-1} + \overline{\overline{I}}/(3\varepsilon_0), \tag{3}$$

where ε_0 is permittivity of free space, $\overline{\overline{I}}$ is unit dyadic. This expression follows from the Lorentz-Lorenz formula

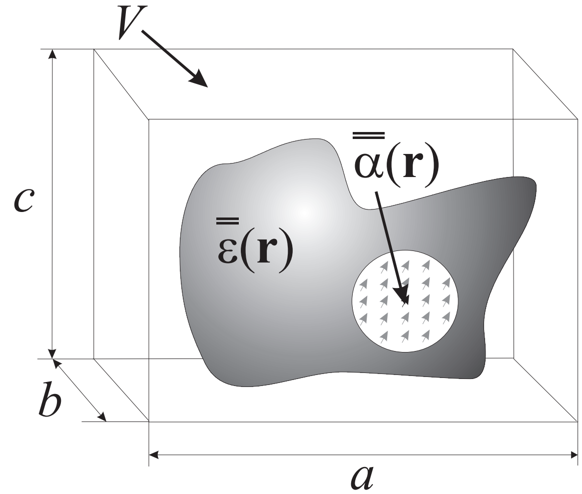

FIG. 2: Illustration for replacement of dielectric permittivity by local polarizability

[9]

$$\mathbf{E}_{\mathrm{loc}}(\mathbf{r}) = \mathbf{E}(\mathbf{r}) + \mathbf{P}(\mathbf{r})/(3\varepsilon_0) \tag{4}$$

and material equation

$$\mathbf{D}(\mathbf{r}) = \varepsilon_0\mathbf{E}(\mathbf{r}) + \mathbf{P}(\mathbf{r}) = \overline{\overline{\varepsilon}}(\mathbf{r})\mathbf{E}(\mathbf{r}). \tag{5}$$

A. Dispersion equation

Following local field approach one can write down dispersion equation for the crystal under consideration in the next integral form:

$$\mathbf{P}(\mathbf{r}) = \overline{\overline{\alpha}}(\mathbf{r}) \int\limits_V \overline{\overline{G}}_3(\mathbf{r} - \mathbf{r}', \mathbf{q})\mathbf{P}(\mathbf{r}')d\mathbf{r}', \ \forall \ \mathbf{r} \in V, \tag{6}$$

where $V = V(\mathbf{a}, \mathbf{b}, \mathbf{c})$ is volume of the elementary lattice cell, $\overline{\overline{G}}_3(\mathbf{r}, \mathbf{q})$ is the lattice dyadic Green's function:

$$\overline{\overline{G}}_3(\mathbf{r}, \mathbf{q}) = \sum_{n,s,l} \overline{\overline{G}}(\mathbf{r} - \mathbf{a}n - \mathbf{b}s - \mathbf{c}l)e^{-j(q_x an + q_y bs + q_z cl)}, \tag{7}$$

which takes into account cell-to-cell polarization distribution determined by wave vector $\mathbf{q} = (q_x, q_y, q_z)^T$:

$$\mathbf{P}(\mathbf{r} + \mathbf{a}n + \mathbf{b}s + \mathbf{c}l) = \mathbf{P}(\mathbf{r})e^{-j(q_x an + q_y bs + q_z cl)}, \tag{8}$$

$\overline{\overline{G}}(\mathbf{r})$ is dyadic Green's function of free space:

$$\overline{\overline{G}}(\mathbf{r}) = (k^2\overline{\overline{I}} + \nabla\nabla)\frac{e^{-jkr}}{4\pi\varepsilon_0 r}, \tag{9}$$

n, s, l are integer indices, k is wave number of free space. The integral in (6) is singular if the point corresponding to vector r is located inside of some polarized dielectric. It has to be evaluated in the meaning of principal value

by excluding small spherical region around the singular point and tending the radius of this region to zero [12].

The dispersion equation (6) relates distribution of polarization density $\mathbf{P}(\mathbf{r})$ and wave vector $\mathbf{q}$ corresponding to the eigenmodes of the electromagnetic crystal. If the distribution of average electric field $\mathbf{E}(\mathbf{r})$ of a crystal eigenmode is known then the polarization density $\mathbf{P}(\mathbf{r})$ can be found directly using material equation (5):

$$\mathbf{P}(\mathbf{r}) = [\overline{\overline{\varepsilon}}(\mathbf{r}) - \varepsilon_0]\mathbf{E}(\mathbf{r}). \tag{10}$$

The reverse operation is possible only for space regions filled by dielectric with $\overline{\overline{\varepsilon}}(\mathbf{r}) \neq \varepsilon_0$. The distribution of electric field in free space regions, if required, have to be calculated using the next integral representation

$$\mathbf{E}(\mathbf{r}) = \int\limits_V \overline{\overline{G}}_3(\mathbf{r}-\mathbf{r}', \mathbf{q})\mathbf{P}(\mathbf{r}')d\mathbf{r}'. \tag{11}$$

For our proof of generalized Ewald-Oseen extinction principle we have to transform dispersion equation (6) into the form corresponding to summation by layers in x-direction. The expression for lattice dyadic Green's function $\overline{\overline{G}}_3(\mathbf{r}, \mathbf{q})$ (7) can be rewritten using summation over planes in the form:

$$\overline{\overline{G}}_3(\mathbf{r}, \mathbf{q}) = \sum_{n=-\infty}^{+\infty} \overline{\overline{G}}_2(\mathbf{r} - \mathbf{a}n)e^{-jq_x an}, \tag{12}$$

where $\overline{\overline{G}}_2(\mathbf{r})$ is the grid dyadic Green's function:

$$\overline{\overline{G}}_2(\mathbf{r}) = \sum_{s,l} \overline{\overline{G}}(\mathbf{r} - \mathbf{b}s - \mathbf{c}l)e^{-j(q_y bs + q_z cl)}. \tag{13}$$

Applying Poisson summation formula by both indices s and l one can express the grid dyadic Green's function in terms of the spatial Floquet harmonics. This expansion is also called as spectral representation:

$$\overline{\overline{G}}_2(\mathbf{r}) = \sum_{s,l} \overline{\overline{\gamma}}_{s,l}^{\,\mathrm{sign}(x-a)} e^{-j(\mathbf{k}_{s,l}^{\mathrm{sign}(x)}\cdot\mathbf{r})}, \tag{14}$$

where

$$\overline{\overline{\gamma}}_{s,l}^{\pm} = \frac{j}{2bc\varepsilon_0 k_{s,l}}[\mathbf{k}_{s,l}^{\pm} \times [\mathbf{k}_{s,l}^{\pm} \times \overline{\overline{I}}]], \;\; \mathbf{k}_{s,l}^{\pm} = (\pm k_{s,l}^x, k_s^y, k_l^z)^T,$$

$$k_s^y = q_y + \frac{2\pi s}{b}, k_l^z = q_z + \frac{2\pi l}{c}, k_{s,l}^x = \sqrt{k^2 - (k_s^y)^2 - (k_l^z)^2}.$$

The square root in the expression for $k_{s,l}$ should be chosen so that $\mathrm{Im}(\sqrt{\cdot}) < 0$. The sign $\pm$ corresponds to half spaces $x > a$ and $x < a$ respectively.

Using (12) the dispersion equation (6) can be rewritten in the following form which will be used later on:

$$\mathbf{P}(\mathbf{r}) = \overline{\overline{\alpha}}(\mathbf{r}) \sum_{n=-\infty}^{+\infty} \int\limits_V \overline{\overline{G}}_2(\mathbf{r} - \mathbf{r}' - \mathbf{a}n)\mathbf{P}(\mathbf{r}')e^{-jq_x an}d\mathbf{r}'. \tag{15}$$

B. Semi-infinite crystal

Now let us consider a semi-infinite crystal (half space $x \geq a$, see Figure 3) excited by a plane electromagnetic wave with wave vector $\mathbf{k} = (k_x, k_y, k_z)^T$ coming from free space:

$$\mathbf{E}_{\mathrm{inc}}(\mathbf{r}) = \mathbf{E}_{\mathrm{inc}}e^{-j(\mathbf{k}\cdot\mathbf{r})}. \tag{16}$$

The origin of our coordinate system is intentionally shifted by one period into the free space since it simplifies rather cumbersome calculations which are presented below and causes exponential convergence of series in the final expressions.

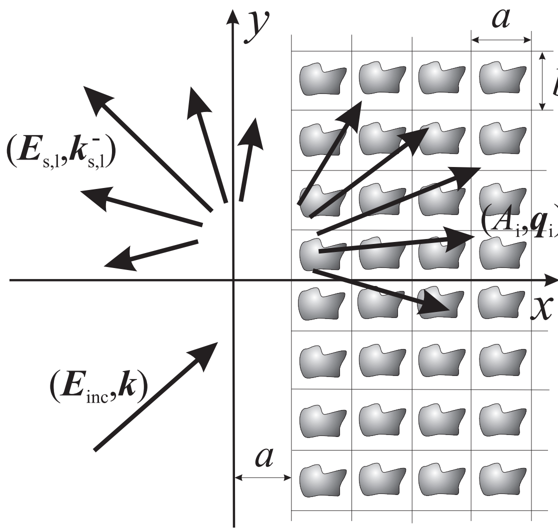

FIG. 3: Geometry of an semi-infinite electromagnetic crystal

Due to the periodicity of the semi-infinite structure along $y-$ and $z-$axes the distribution of the excited polarization along these directions is determined by the phase of the incident wave:

$$\mathbf{P}(\mathbf{r} + \mathbf{a}m + \mathbf{b}s + \mathbf{c}l) = \mathbf{P}(\mathbf{r} + \mathbf{a}m)e^{-j(k_y bn + k_z cl)}, \tag{17}$$

for any $\mathbf{r} \in V$ and $m \geq 1$.

The electric field produced by the polarized semi-infinite crystal has the form

$$\mathbf{E}_{\mathrm{scat}}(\mathbf{r}) = \sum_{n=1}^{+\infty} \int\limits_V \overline{\overline{G}}_2(\mathbf{r} - \mathbf{r}' - \mathbf{a}n)\mathbf{P}(\mathbf{r}' + \mathbf{a}n)d\mathbf{r}'. \tag{18}$$

The total local electric field is sum of incident and scattered (produced by polarization of crystal) fields. Following the local field approach we can write:

$$\mathbf{P}(\mathbf{r}) = \overline{\overline{\alpha}}(\mathbf{r})\left[\mathbf{E}_{\mathrm{inc}}(\mathbf{r}) + \mathbf{E}_{\mathrm{scat}}(\mathbf{r})\right]. \tag{19}$$

Combining (18) and (19) we obtain an integral equation for the polarization in the semi-infinite crystal ex-

cited by an incident wave:

$$\mathbf{P}(\mathbf{r}) = \overline{\overline{\alpha}}(\mathbf{r}) \left[\mathbf{E}_{\mathrm{inc}}(\mathbf{r}) + \sum_{n=1}^{+\infty} \int\limits_V \overline{\overline{G}}_2(\mathbf{r} - \mathbf{r}' - \mathbf{a}n) \mathbf{P}(\mathbf{r}' + \mathbf{a}n) d\mathbf{r}' \right]. \tag{20}$$

Now let us suppose that the dispersion equation (6) is solved under condition that wave vector has the form $\mathbf{q} = (q_x, k_y, k_z)^T$ with unknown $x-$component q_x, and the set of eigenmodes $\{(\mathbf{P}_i(\mathbf{r}), q_x^{(i)})\}$, characterized by x-component of wave vector $q_x^{(i)}$ and polarization distribution $\mathbf{P}_i(\mathbf{r})$, is found. In addition, we include into this set only the eigenmodes which either transfer energy into half-space $x \geq a$ $[dq_x^{(i)}/d\omega > 0]$ or decay in x-direction $[\mathrm{Im}(q_x^{(i)}) < 0]$. In such a case the polarization of the semi-infinite crystal excited by the incident wave (16) can be expanded by the eigenmodes of infinite crystal as follows:

$$\mathbf{P}(\mathbf{r} + \mathbf{a}m) = \sum_i A_i \mathbf{P}_i(\mathbf{r}) e^{-jq_x^{(i)} am}, \ \forall \mathbf{r} \in V, m \geq 1. \tag{21}$$

Substituting (21) into (20) and using (16) we obtain:

$$\sum_i A_i \mathbf{P}_i(\mathbf{r}) e^{-jq_x^{(i)} am} = \overline{\overline{\alpha}}(\mathbf{r}) \left[\mathbf{E}_{\mathrm{inc}} e^{-j\mathbf{k}(\mathbf{r}+\mathbf{a}m)} \right. \tag{22}$$

$$\left. + \sum_{n=1}^{+\infty} \sum_i A_i \int\limits_V \overline{\overline{G}}_2(\mathbf{r} - \mathbf{r}' - \mathbf{a}(n-m)) \mathbf{P}_i(\mathbf{r}') e^{-jq_x^{(i)} an} d\mathbf{r}' \right].$$

Splitting series in the dispersion equation (15) one can derive the following auxiliary relation:

$$\mathbf{P}_i(\mathbf{r}) e^{-jq_x^{(i)} am} =$$

$$= \overline{\overline{\alpha}}(\mathbf{r}) \sum_{n=1}^{+\infty} \int\limits_V \overline{\overline{G}}_2(\mathbf{r} - \mathbf{r}' - \mathbf{a}(n-m)) \mathbf{P}_i(\mathbf{r}') e^{-jq_x^{(i)} an} d\mathbf{r}' \tag{23}$$

$$+ \overline{\overline{\alpha}}(\mathbf{r}) \sum_{n=-\infty}^{0} \int\limits_V \overline{\overline{G}}_2(\mathbf{r} - \mathbf{r}' - \mathbf{a}(n-m)) \mathbf{P}_i(\mathbf{r}') e^{-jq_x^{(i)} an} d\mathbf{r}'.$$

Substituting (23) into (22) and following the fact that $\det\{\overline{\overline{\alpha}}(\mathbf{r})\} \neq 0$ we obtain:

$$\sum_i A_i \sum_{n=-\infty}^{0} \int\limits_V \overline{\overline{G}}_2(\mathbf{r} - \mathbf{r}' - \mathbf{a}(n-m)) \mathbf{P}_i(\mathbf{r}') e^{-jq_x^{(i)} an} d\mathbf{r}'$$

$$= \mathbf{E}_{\mathrm{inc}} e^{-j\mathbf{k}(\mathbf{r}+\mathbf{a}m)}. \tag{24}$$

Further, substituting (14) into (24), changing the summation order and evaluating the sum of the geometrical progression by index n we get:

$$\sum_{s,l} \left(\sum_i A_i \frac{\overline{\overline{\gamma}}^+_{s,l} \int\limits_V \mathbf{P}_i(\mathbf{r}') e^{j(\mathbf{k}^+_{s,l} \cdot \mathbf{r}')} d\mathbf{r}'}{1 - e^{j(q_x^{(i)} - k^x_{s,l})a}} \right) e^{-j(\mathbf{k}^+_{s,l} \cdot (\mathbf{r}+\mathbf{a}m))}$$

$$= \mathbf{E}_{\mathrm{inc}} e^{-j\mathbf{k}(\mathbf{r}+\mathbf{a}m)}. \tag{25}$$

C. Generalized Ewald-Oseen extinction principle

The left part of equation (25) represents an expansion of the right part into a spatial spectrum of Floquet harmonics. The right part represents an incident spectrum of Floquet harmonics containing only the single incident plane wave (16) with $\mathbf{k} = \mathbf{k}^+_{0,0}$. Equating coefficients in the left and right parts of (25) we obtain:

$$\overline{\overline{\gamma}}^+_{s,l} \sum_i A_i \frac{\int\limits_V \mathbf{P}_i(\mathbf{r}') e^{j(\mathbf{k}^+_{s,l} \cdot \mathbf{r}')} d\mathbf{r}'}{1 - e^{j(q_x^{(i)} - k^x_{s,l})a}} = \begin{cases} \mathbf{E}_{\mathrm{inc}}, \ (s,l) = (0,0) \\ 0, \ (s,l) \neq (0,0) \end{cases}. \tag{26}$$

The values in the right side of (26) are the amplitudes of the incident spatial harmonics (all harmonics except fundamental one have zero amplitudes), and the series in the left side are the amplitudes of the spatial harmonics produced by the whole semi-infinite crystal polarization in order to cancel these incident harmonics. It means that equation (26) represents the generalization of Ewald-Oseen extinction principle (see [7–9] for classical formulation in the case of dielectrics): *the polarization in a semi-infinite electromagnetic crystal excited by a plane wave is distributed in such a way that it cancels the incident wave together with all high-order spatial harmonics associated with periodicity of the boundary* (even if they have zero amplitudes as in the present case). The additional words related to high-order Floquet harmonics is the main and principal difference of Ewald-Oseen extinction principle formulation for electromagnetic crystals as compared to the classical case of isotropic dielectrics.

Substitution of (21) and (14) into (18) allows to express the scattered field in the half space $x < a$ in terms of spatial Floquet harmonics:

$$\mathbf{E}_{\mathrm{scat}} = \sum_{s,l} \mathbf{E}^{s,l}_{\mathrm{scat}} e^{-j(\mathbf{k}^-_{s,l} \cdot \mathbf{r})}, \tag{27}$$

$$\mathbf{E}^{s,l}_{\mathrm{scat}} = \overline{\overline{\gamma}}^-_{s,l} \sum_i A_i \frac{\int\limits_V \mathbf{P}_i(\mathbf{r}') e^{j(\mathbf{k}^-_{s,l} \cdot \mathbf{r}')} d\mathbf{r}'}{1 - e^{j(q_x^{(i)} + k^x_{s,l})a}}. \tag{28}$$

Note, that the formula for the amplitudes of scattered Floquet harmonics (28) contains series which have the same form as (26) and differs only by the sign of the

$x-$ components of wave vectors $\mathbf{k}^{\pm}_{s,l} = (\pm k^x_{s,l}, k_y, k_z)^T$ corresponding to the spatial harmonics propagating into the half spaces $x < a$ and $x > a$, respectively.

If the eigenmodes of the crystal $\{q_x^{(i)}, \mathbf{P}_i(\mathbf{r})\}$ are known then one can solve the system of linear equations (26) and find amplitudes of excited eigenmodes $\{A_i\}$. With use of these amplitudes the scattered field can be found by (28). This provides a new numerical method which allows to solve problem of plane-wave diffraction by a semi-infinite electromagnetic crystal using knowledge of eigenmodes of the infinite crystal. This fact is very important since at the moment the reflection and dispersion problems for electromagnetic crystals are usually solved by separate numerical approaches. The expressions (26) and (28) create a link between these two problems and show how results of dispersion studies can be used in order to describe reflection properties of electromagnetic crystals.

Until this point we considered only one incident wave with wave vector $\mathbf{k} = \mathbf{k}^+_{0,0}$, but from (25) it is clear that we could consider also other incident spatial harmonics with wave vectors $\mathbf{k}^+_{s,l}$ and get the similar results as (26), but the nonzero terms at the right side of equation would correspond to the respective incident spatial harmonic. Using principle of superposition we obtain that if the semi-infinite crystal is excited by whole spectrum of incident spatial harmonics with amplitudes $\mathbf{E}^{s,l}_{\text{inc}}$ and wave vectors $\mathbf{k}^+_{s,l}$ then the following system of linear equations is valid:

$$\overline{\overline{\gamma}}^+_{s,l} \sum_i A_i \frac{\int\limits_V \mathbf{P}_i(\mathbf{r'}) e^{j(\mathbf{k}^+_{s,l}\cdot\mathbf{r'})} d\mathbf{r'}}{1 - e^{j(q_x^{(i)} - k^x_{s,l})a}} = \mathbf{E}^{s,l}_{\text{inc}} \tag{29}$$

The scattered field is given by (28) as in the case of one incident wave. The equation (29) represents cancelation of all incident spatial spectrum by induced polarization of the crystal in accordance to the formulated above generalized Ewald-Oseen extinction principle.

D. Formulation of boundary conditions

In the previous section we have proved generalized Ewald-Oseen extinction principle for the case of semi-infinite electromagnetic crystal described by certain periodic permittivity distribution $\overline{\overline{\varepsilon}}(\mathbf{r})$ excited by a plane wave coming from free space. In order to extend this theory for the case when incident wave comes from homogeneous isotropic dielectric with permittivity ϵ it is enough to change ϵ_0 in all formulae to ϵ. Physically it means that we have to consider the polarization of the crystal with respect to the host material with permittivity ε, but not free space. In the model of dense cubic lattice of point dipoles it means that the lattice is located inside of this host material. This approach is very unusual since it can lead to results which are strange from first point of view. For example, free space happen to have negative polarization density with respect to dielectrics with $\varepsilon > \varepsilon_0$. This can be simply explained since free space with respect to these dielectrics is like real materials with $\varepsilon < \varepsilon_0$ with respect to free space: they indeed have negative polarization density.

The meaning of polarization density becomes relative automatically when the replacement of ε_0 to ε is made. In order to avoid the use of this ambiguous polarization in the final formulae it is possible to express the polarization density in terms of the average field using (5). The resulting expressions provide complete set of boundary conditions for interface between semi-infinite electromagnetic crystal and isotropic dielectric:

$$\mathbf{E}(\mathbf{r}) = \begin{cases} \sum\limits_{s,l} \left(\mathbf{E}^{s,l}_{\text{inc}} e^{-j\mathbf{k}^-_{s,l}\mathbf{r}} + \mathbf{E}^{s,l}_{\text{scat}} e^{-j\mathbf{k}^+_{s,l}\mathbf{r}} \right), \ x < a \\ \sum\limits_i A_i \mathbf{E}_i e^{-j\mathbf{q}_i\mathbf{r}}, \ x \geq a \end{cases} \tag{30}$$

$$\overline{\overline{\gamma}}^+_{s,l} \sum_i A_i \frac{\int\limits_V [\overline{\overline{\varepsilon}} - \varepsilon_0 \overline{\overline{I}}] \mathbf{E}_i(\mathbf{r'}) e^{j(\mathbf{k}^+_{s,l}\cdot\mathbf{r'})} d\mathbf{r'}}{1 - e^{j(q_x^{(i)} - k^x_{s,l})a}} = \mathbf{E}^{s,l}_{\text{inc}}, \tag{31}$$

$$\overline{\overline{\gamma}}^-_{s,l} \sum_i A_i \frac{\int\limits_V [\overline{\overline{\varepsilon}} - \varepsilon_0 \overline{\overline{I}}] \mathbf{E}_i(\mathbf{r'}) e^{j(\mathbf{k}^-_{s,l}\cdot\mathbf{r'})} d\mathbf{r'}}{1 - e^{j(q_x^{(i)} + k^x_{s,l})a}} = \mathbf{E}^{s,l}_{\text{scat}}, \tag{32}$$

where we use following notations

$$\overline{\overline{\gamma}}^\pm_{s,l} = \frac{j}{2bc\varepsilon k_{s,l}} [\mathbf{k}^\pm_{s,l} \times [\mathbf{k}^\pm_{s,l} \times \overline{\overline{I}}]], \ \mathbf{k}^\pm_{s,l} = (\pm k^x_{s,l}, k^y_s, k^z_l)^T,$$

$$k^y_s = q_y + \frac{2\pi s}{b}, k^z_l = q_z + \frac{2\pi l}{c}, k^x_{s,l} = \sqrt{k^2 - (k^y_s)^2 - (k^z_l)^2},$$

k is wave number in the dielectric with permittivity ε, $\mathbf{q}_i = (q^x_i, k_y, k_z)^T$ and the square root in the expression for $k_{s,l}$ should be chosen so that $\mathrm{Im}(\sqrt{\cdot}) < 0$.

The expressions (31) and (32) relate amplitudes of incident $\mathbf{E}^{s,l}_{\text{inc}}$ and scattered $\mathbf{E}^{s,l}_{\text{scat}}$ spatial harmonics corresponding to tangential wave vector $\mathbf{k}_t = (k_y, k_z)^T$ and periodicity of the boundary (rectangular lattice with periods b and c) with amplitudes A_i of eigenmodes $(\mathbf{E}_i, q^x_i)$ excited in the semi-infinite crystal.

The presented set of boundary conditions is complete: these equations are enough to determine amplitudes of excited eigenmodes and scattered spatial harmonics if the eigenmodes $\{(\mathbf{E}_i, q^x_i)\}$ of infinite crystal corresponding to tangential wave vector $\mathbf{k}_t$ are known. But this set is not unique. One can immediately suggest to use classical boundary conditions (continuous tangential component of electric field and normal component of electric displacement at any point of the boundary $x = a$) which being expanded into Fourier series will also grant a complete set of linear equations relating amplitudes of incident, scattered and excited modes.

The advantage of equations (31) and (32) as compared to any other boundary conditions is such that they have very special form which can admit analytical solution. We will demonstrate it in the next section for the special case of electromagnetic crystals formed by small scatterers which can be treated as point dipole with fixed orientation. But this is not the only case when an analytical solution of (31) and (32) can be obtained. Recently, M. Silveirinha [13] demonstrated that the method proposed by ourselves can be successfully applied for studies of reflection from semi-infinite wire medium, material with strong low-frequency spatial dispersion [14]. Unfortunately, we can not provide solution of equations (31) and (32) for the general case. However, we can give some recommendations and an example how these equations can be solved using method of characteristic function. We hope that with some modification this method can be used for other special cases as well.

III. LATTICE OF UNIAXIAL DIPOLAR SCATTERERS

If the scatterers which form electromagnetic crystal are small as compared to the wavelength then sometimes they can be effectively replaced by point dipoles. It is assumed that the dipole moment of such a dipole is determined by local field acting to the scatterer and the field produced by the scatterer is equal to the field created by the dipole. The polarizability which relates the induced dipole moment and the local field acting to the scatterer is the only parameter which depends on the shape of scatterer in such a local field approach.

Generally, the field produced by any scatterer can be presented using expansion by multipoles. The electric and magnetic dipoles are first and second order multipoles. For some scatterers, the electric or magnetic dipole moments dominate over high-order multipoles. It means that some scatterers behave as electrical dipoles, some other ones as magnetic. Below we will consider only such scatterers. The scatterers which has both electric and magnetic dipole moments of the same order or whose quadrupole or other high-order multipoles can not be neglected are out of scope of our consideration. Moreover, below we will consider only scatterers which can be replaced by dipoles with fixed orientation.

The typical example of the scatterer which behaves as electric dipole with fixed orientation at microwave frequencies is a short metallic cylinder or piece of wire which can be loaded by some inductance in order to increase its polarizability [15] (see Fig. 4.b). At optical frequencies it can be prolate metallic cylinder which has strong plasmonic resonance. The typical magnetic scatterer at microwave frequencies is split-ring resonator [16] (see Fig. 4.a) if the bianisotropic properties of this scatterer are neglected or canceled using method suggested in [17]. At optical frequencies the split metallic rings [18, 19] behave as magnetic scatterers with fixed orientation of dipole moment. Metallic spheres which also can be replaced by point dipoles are out of scope of our consideration since the orientation of their dipole moments depends on direction of external field.

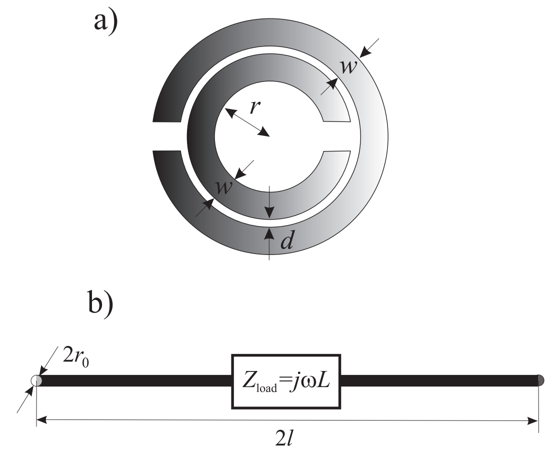

FIG. 4: Geometries of scatterers which can be modeled as dipoles with fixed orientation: a) split-ring-resonator, b) inductively loaded wire.

A. History of the problem

Further in this section we present an analytical solution for problem of plane wave diffraction on semi-infinite electromagnetic crystals formed by point scatterers with known polarizabilites, but before that we have to describe history of this problem. The first attempt to obtain such an analytical solution has been made by G.D. Mahan and G. Obermair in a seminal work [10]. Analytical expressions for reflection coefficients and amplitudes of excited modes for a semi-infinite crystal were obtained in terms of wave vectors of the infinite crystal eigenmodes. However this theory is not free from the drawbacks. Mahan and Obermair treated the interaction between a reference crystal plane of a semi-infinite crystal and its N nearest neighbors exactly, neglecting the other crystal planes. That is why this approximation is called "near-neighbor approximation". Such an approach allows to introduce fictitious zero polarization at the imaginary crystal planes in free space over the semi-infinite crystal. This manipulation gave a set of equations which were treated in [10] as additional boundary conditions. It will be shown below that if the interaction between planes is taken into account exactly but not restricted to finite number of neighboring planes then the fictitious polarization of imaginary planes turns out to be non-zero. In works of C.A. Mead [20, 21] it was already shown that the "near-neighbor approximation" appears to be not a strict one. The mead states that the serious disagreement appears in the cases then the interaction between crystal planes falls off not sufficiently fast with distance. In other words, the results of Mahan and Obermair are valid

only then the high-order spatial Floquet harmonics produced by the planes rapidly decay with distance. Mahan and Obermair considered only the normal incidence of the plane wave. Within such a restriction their approach is valid in the case when the periods of the structure are small as compared with the wavelength in the host medium. The strong disagreement with the exact solution appears when one of high-order Floquet harmonic happens to be propagating one. This fact is illustrated below by a numerical comparison.

The work [10] caused numerous extensions [22–24]. The Mahan and Obermair approach was generalized for the cases of oblique incidence [22], both possible polarizations of incident wave [24], various lattice structures of the crystal [22], tensorial polarizability of scatterers [24] and even diffraction of the finite-size slabs of the crystals was considered [23]. Note, that all the listed works use the same "near-neighbor approximation" and their applicability is restricted as described above. In order to avoid this trouble one needs to use another model for interaction between crystal planes. The simplest one is the so-called "exp model" suggested by Mead [20, 25] which assumes that interaction can be described by a single decaying exponent. In terms of spatial Floquet harmonics this approach is equivalent to neglecting all high-order Floquet harmonics except the one with the slowest decay. The "exp model" as well as the "near-neighbor approximation" allow to solve the problem of excitation analytically for both normal [20] and oblique [25] incidences. The "exp model" of Mead gives a set of two equations which correspond to the generalized Ewald-Oseen extinction principle formulated in the present paper. The first equation of Mead is the same as one of equations given by "near-neighbor approximation". It describes the fact that the incident electromagnetic wave (fundamental Floquet harmonic) inside the semi-infinite crystal is canceled by induced polarization of the crystal. This fact was pointed out in the papers [10, 20, 24]. The second equation clearly expresses the fact that induced polarization cancels also the second Floquet harmonic (taken into account in the "exp model") of incident wave which has zero amplitude, but unfortunately it was not noted by the authors. The system of these two equations is solved in [20] and the amplitudes of excited eigenmodes and an expression for reflection coefficient are obtained.

It is possible to modify the "exp model" in order to obtain an exact solution. For that purpose one simply should take into account all Floquet harmonics in the interaction between the crystal planes. This has been done by authors of the present paper and the results are presented below. As it was shown above, it turns out that every incident Floquet harmonic (even if it has zero amplitude) is canceled by the induced polarization following to the generalized Ewald-Oseen extinction principle. It provides an infinite system of equations relating amplitudes of excited eigenmodes. This system can be truncated and then the number of equations in the system turns out to be equal to the number of Floquet harmonics taken into account. Such the finite system can be easily solved analytically for the case when only two Floquet harmonics are taken into account (this is the "exp model" of Mead [20]), but in the case when one would like to take into account more Floquet harmonics this approach requires numerical calculations. We avoid the truncation of the system of equations and offer a closed-form rigorous analytical solution which is simple and explicit.

Note, that a "formally closed solution" for the problem under consideration was proposed by Mead in [21]. In this solution there is a contour integral of a certain function given in the form of infinite series. However, the calculation with help of such "formally closed solution" requires serious numerical efforts. The main idea of work [21] is based on introduction of characteristic analytical function which allows to determine all parameters entering the expression for the reflection coefficient. It is shown that knowledge of its roots allows to recover this function and obtain analytical expressions for all amplitudes of excited eigenmodes and for the reflection coefficient, consequently. Unfortunately, these roots were not found in [21]. That is why the contour integration was used in [21] in order to bypass the problem of these roots finding. In fact, as it is shown below, the roots of this characteristic analytical function are determined by the wave vectors of Floquet harmonics and can be easily expressed analytically. This fact is a consequence of generalized Ewald-Oseen extinction principle which is an important point of our theory.

One could directly apply general results (26) and (28) to the problem under consideration. It is enough to replace polarization density of eigenmodes by three-dimensional delta function corresponding to the point of location of the dipolar scatterer in the unit cell and one could obtain the system of linear equations (26) and (28) which correspond to the boundary conditions in the present case as it is shown below. However, we prefer to re-deduce all the expressions by making the same steps as in the previous section but for the case of point scatterers. We suppose that it is very useful step in order to demonstrate physical background of the computations undertaken in the previous section at a specific example.

B. Dispersion equation

Let us consider an infinite crystal formed by point dielectric dipoles with some known polarizability α along fixed direction given by unit vector $\mathbf{d}$, $\overline{\overline{\alpha}} = \alpha\mathbf{d}\mathbf{d}$. The case of magnetic dipoles can be easily obtained from the theory for dielectric ones using duality principle. The scatterers are arranged in the nodes of the three-dimensional lattice with an orthorhombic elementary cell $a \times b \times c$ located in free space, see Figure 5.

The distribution of dipole moments corresponding to an eigenmode with wave vector $\mathbf{q} = (q_x, q_y, q_z)^T$ is described as $\mathbf{p}_{n,s,l} = \mathbf{p}e^{-j(q_x an + q_y bs + q_z cl)}$, where n, s, l are integer indices of scatterers along the $x-, y-, z-$ axes,

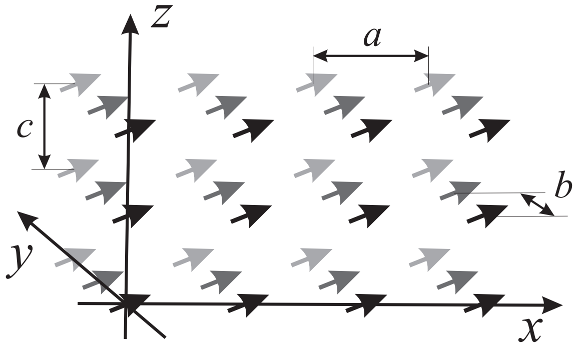

FIG. 5: Geometry of an infinite electromagnetic crystal formed by uniaxial dipolar scatterers

respectively, and $\mathbf{p}$ is a dipole moment of the scatterer located at the center of coordinate system. Following to the local field approach $\mathbf{p}$ can be expressed as $\mathbf{p} = \alpha(\mathbf{E}_{\text{loc}} \cdot \mathbf{d})\mathbf{d}$, where $\mathbf{E}_{\text{loc}}$ is a local electric field acting to the scatterer. The local field is produced by all other scatterers which form the infinite crystal and it can be given by the formula

$$\mathbf{E}_{\text{loc.}} = \sum_{n,s,l}{}' \overline{\overline{G}}(\mathbf{R}_{n,s,l})\mathbf{p}_{n,s,l}, \tag{33}$$

where $\overline{\overline{G}}(\mathbf{r})$ is the three-dimensional dyadic Green function of the free space (9) and summation is taken over all triples of indices except the zero one. Accordingly the following dispersion equation for the crystal under consideration is obtained (compare with (6)):

$$\alpha^{-1} = \left[\sum_{n,s,l}{}' \overline{\overline{G}}(\mathbf{R}_{n,s,l})e^{-j(q_x an + q_y bs + q_z cl)}\mathbf{d}\right] \cdot \mathbf{d}. \tag{34}$$

In order to evaluate sums of series in (34) we use a plane-wise approach [26]. According to this approach the dispersion equation takes the following form:

$$\alpha^{-1} = \sum_{n=-\infty}^{+\infty} \beta_n e^{-jq_x an}. \tag{35}$$

The coefficients β_n describe the interaction between planes and include the information on transverse wave vector components q_y, q_z as well as on a geometry of a single plane (lattice periods b, c). For $n \neq 0$ coefficients β_n can be expressed using expansion by Floquet harmonics. For $n = 0$ the calculation of coefficient β_0 (describing interaction inside of a plane and expressed in the form of two-dimensional series without the zero term) requires additional efforts (see [11, 26, 27] for details).

The electric field produced by a single plane (namely two-dimensional grid $b \times c$ of point dipoles with the distribution $\mathbf{p}_{s,l} = \mathbf{p}e^{-j(q_y bs + q_z cl)}$) located in the plane $x = 0$ is equal to

$$\mathbf{E}(\mathbf{r}) = \frac{j}{2bc\varepsilon_0} \sum_{s,l} [\mathbf{k}_{s,l}^{\text{sign}(x)} \times [\mathbf{k}_{s,l}^{\text{sign}(x)} \times \mathbf{p}]] \frac{e^{-j(\mathbf{k}_{s,l}^{\text{sign}(x)} \cdot \mathbf{R})}}{k_{s,l}^x}, \tag{36}$$

where $\mathbf{k}_{s,l}^{\pm} = (\pm k_{s,l}^x, k_s^y, k_l^z)^T$, $k_s^y = q_y + \frac{2\pi s}{b}$, $k_l^z = q_z + \frac{2\pi l}{c}$, $k_{s,l}^x = \sqrt{k^2 - (k_s^y)^2 - (k_l^z)^2}$ and$k$ is wave number of free space. One should choose the square root in the expression for $k_{s,l}$ so that $\text{Im}(\sqrt{\cdot}) < 0$. The sign $\pm$ corresponds to half spaces $x > 0$ and $x < 0$ respectively.

The formula (36) defines an expansion of the field produced by a single grid of dipoles in terms of plane waves and it can be obtained using double Poisson summation formula to series of fields produced by single scatterers in free space. These plane waves have wave vectors $\mathbf{k}_{s,l}^{\pm}$. They are also called Floquet harmonics and represent a spatial spectrum of the field (compare with (14)). Floquet harmonics are widely used in analysis of phased array antennas [28].

Using (36) we get the following expression for β_n ($n \neq 0$):

$$\beta_n = \sum_{s,l} \gamma_{s,l}^{-\text{sign}(n)} e^{-jk_{s,l}^x a|n|}, \tag{37}$$

where $\gamma_{s,l}^{\pm} = [k^2 - (\mathbf{k}_{s,l}^{\pm} \cdot \mathbf{d})^2]/(2jbc\varepsilon_0 k_{s,l}^x)$. After substitution of (37) into (35), changing the order of summation and using the formula for sum of geometrical progression we obtain the dispersion equation in the following form:

$$\alpha^{-1} = \beta_0 + \sum_{s,l} \left[\frac{\gamma_{s,l}^-}{e^{j(k_{s,l}^x + q_x)a} - 1} + \frac{\gamma_{s,l}^+}{e^{j(k_{s,l}^x - q_x)a} - 1}\right]. \tag{38}$$

This is a transcendental equation expressed by rapidly convergent series. Dispersion properties of the crystal under consideration can be studied with help of numerical solution of the latter equation. The case of dipoles oriented along one of the crystal axes of the orthorhombic crystal has been considered in [11], the dispersion equation was solved and typical dispersion curves and iso-frequency contours for resonant scatterers were presented.

C. Semi-infinite crystal

Now let us consider a semi-infinite electromagnetic crystal, the half-space $x \geq a$ filled by the crystal formed by point dipoles, see Figure 6. The structure is excited by a plane electromagnetic wave with the wave vector $\mathbf{k} = (k_x, k_y, k_z)^T$ and the intensity of electric field $\mathbf{E}_{\text{inc}}$. Let us denote the component of the incident electric field along the direction of dipoles as $E_{\text{inc}} = (\mathbf{E}_{\text{inc}} \cdot \mathbf{d})$. The axis x is assumed to be normal to the interface. The tangential (with respect to the interface) distribution of dipole moments in excited semi-infinite crystal is determined by the tangential component of the incident wave

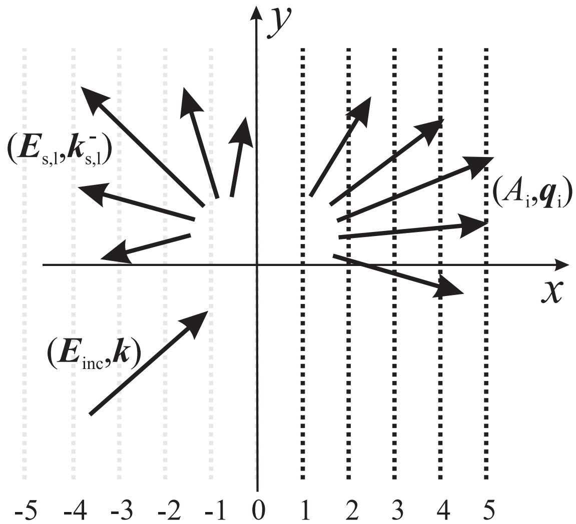

FIG. 6: Geometry of a semi-infinite electromagnetic crystal formed by uniaxial dipolar scatterers

vector. It means that $p_{n,s,l} = p_n e^{-j(k_y bs + k_z cl)}$, where the polarizations of zero-numbered scatterers from planes with the index n (parallel to the interface) are denoted as $p_n = p_{n,0,0}$. The plane-to-plane distribution $\{p_n\}$ is unknown and it has to be found. Using the local field approach one can write the infinite linear system of equations for this distribution:

$$p_m = \alpha \left(E_{\mathrm{inc}} e^{-jk_x am} + \sum_{n=1}^{+\infty} \beta_{n-m} p_n \right), \ \forall\ m \geq 1. \quad (39)$$

The distribution $\{p_n\}$ of polarization in the excited semi-infinite crystal can be determined solving the system of equations (39). The known distribution of polarization allows to determine the scattered field in the half-space $x < a$ with help of the expansion by Floquet harmonics (36):

$$\mathbf{E} = \sum_{s,l} \mathbf{E}_{s,l} e^{-j(\mathbf{k}^-_{s,l}\cdot\mathbf{R})}, \quad (40)$$

where the amplitudes of Floquet harmonics are following:

$$\mathbf{E}_{s,l} = \frac{j}{2ab\varepsilon_0 k^x_{s,l}} [\mathbf{k}^-_{s,l} \times [\mathbf{k}^-_{s,l} \times \mathbf{d}]] \sum_{n=1}^{+\infty} p_n e^{-jk^x_{s,l} an}. \quad (41)$$

If the crystal supports propagating modes, it is quite difficult to find a solution of (39) numerically. Simple methods such as system truncating (considering a slab with finite thickness instead of half-space like in [29]) results in nonconvergent oscillating solutions which have nothing to do with actual solution of (39).

D. Expansion by eigenmodes

In order to solve (39) accurately one has to use an expansion of the polarization by eigenmodes [10]:

$$p_n = \sum_i A_i e^{-jq^{(i)}_x an}, \quad (42)$$

where A_i are amplitudes of eigenmodes and $q^{(i)}_x$ are the x-components of their wave vectors. Every eigenmode is assumed to be a solution of the dispersion equation (38) with the wave vector $\mathbf{q}_i = (q^{(i)}_x, k_y, k_z)^T$. In the formula (42) the summation is taken by eigenmodes which either transfer energy into half-space $x \geq a$ ($\frac{dq^{(i)}_x}{d\omega} > 0$) or decay along $x-$axis ($\mathrm{Im}(q^{(i)}_x) < 0$).

Let us assume that the dispersion equation (38) is solved (for example numerically) and the necessary set of eigenmodes $\{q^{(i)}_x\}$ is found. Then the substitution of (42) into (39) will replace the set of unknown polarizations of planes by a set of unknown amplitudes of eigenmodes:

$$\alpha^{-1} \sum_i A_i e^{-jq^{(i)}_x am} = E_{\mathrm{inc}} e^{-jk_x am} + \sum_{n=1}^{+\infty} \beta_{n-m} \sum_i A_i e^{-jq^{(i)}_x an}. \quad (43)$$

Applying the auxiliary relation evidently following from (38):

$$\alpha^{-1} e^{-jq^{(i)}_x am} - \sum_{n=-\infty}^{0} \beta_{n-m} e^{-jq^{(i)}_x an} = \sum_{n=1}^{+\infty} \beta_{n-m} e^{-jq^{(i)}_x an}, \quad (44)$$

the equation (43) can be transformed as follows:

$$\sum_i A_i \left(\sum_{n=-\infty}^{0} \beta_{n-m} e^{-jq^{(i)}_x an} \right) = E_{\mathrm{inc}} e^{-jk_x am}. \quad (45)$$

It should be noted, that using definition of Mahan and Obermair for the polarization of fictitious planes ($p_n = \sum_i A_i e^{-jq^{(i)}_x an}$, $\forall n \leq 0$) one can rewrite (45) as

$$\sum_{n=-\infty}^{0} \beta_{n-m} p_n = E_{\mathrm{inc}} e^{-jk_x am}. \quad (46)$$

It is evident that the assumption of Mahan and Obermair, requiring all polarizations of fictitious planes to be zeros, contradicts with (46). This fact proves that the "near-neighbor approximation" made in [10] is not accurate.

The system of equations (45) can be truncated and solved numerically quite easily in contrast to (39). As a result, the amplitudes of eigenmodes $\{A_i\}$ can be found and the polarization distribution can be restored using formula (42). The amplitudes of scattered Floquet harmonics (41) can be also expressed in terms of excited eigenmodes amplitudes by means of substitution of (42)

into (41), changing the order of summation and evaluating sums of geometrical progressions. The final expression for the amplitudes of scattered Floquet harmonics is following (compare with (28)) :

$$\mathbf{E}_{s,l} = \frac{[\mathbf{k}_{s,l}^{-} \times [\mathbf{k}_{s,l}^{-} \times \mathbf{d}]]}{2jab\varepsilon_0 k_{s,l}^x} \sum_i A_i \frac{1}{1 - e^{j(q_x^{(i)} + k_{s,l}^x)a}}. \quad (47)$$

One can stop at this stage and claim that the problem of the semi-infinite electromagnetic crystal excitation is solved. However in this case the solution would require long numerical calculations, such as solving the system (45) and substituting the obtained solution into (47). The possibility to make all described operations analytically in the closed-form is shown below.

E. Analytical solution

Substituting the expansion (37) into (45) we obtain:

$$\sum_i A_i \left(\sum_{n=-\infty}^{0} \left[\sum_{s,l} \gamma_{s,l}^{+} e^{-jk_{s,l}^x a|n-m|} \right] e^{-jq_x^{(i)} an} \right)$$

$$= E_{\text{inc}} e^{-jk_x am}. \quad (48)$$

Changing the order of summation in (48), taking into account that $n - m < 0$ and using formula for the sum of geometrical progression we obtain:

$$\sum_{s,l} \gamma_{s,l}^{+} \left(\sum_i A_i \frac{1}{1 - e^{j(q_x^{(i)} - k_{s,l}^x)a}} \right) e^{-jk_{s,l}^x am} = E_{\text{inc}} e^{-jk_x am} \quad (49)$$

This is a system of linear equations where unknowns are given by expressions in brackets. It has a unique solution because the determinant of the system has finite nonzero value. Note that $k_{s,l}^x = k_x$ only if $(s,l) = (0,0)$. Thus, the solution of (49) has the following form:

$$\sum_i A_i \frac{1}{1 - e^{j(q_x^{(i)} - k_{s,l}^x)a}} = \begin{cases} E_{\text{inc}}/\gamma_{0,0}^{+}, \text{ if } (s,l) = (0,0) \\ 0, \text{ if } (s,l) \neq (0,0) \end{cases} \quad (50)$$

This equation could be directly obtained from general expression (26) by substitution of delta function instead of polarization density of eigenmodes, but as we already mentioned above we intentionally re-deduced it since we suppose that it can help to understand background for deduction of (26) for general case. The values at the right side of (50) are the normalized amplitudes of incident Floquet harmonics, and the series at the left side are the normalized amplitudes of Floquet harmonics produced by the whole semi-infinite crystal polarization which cancel the incident harmonics. Thus, the equation (50) represents the generalization of the Ewald-Oseen extinction principle already formulated above for general case of semi-infinite crystals: *The polarization in a semi-infinite electromagnetic crystal excited by a plane wave is distributed in such a way that it cancels the incident wave together with all high-order spatial harmonics associated with periodicity of the boundary.*

Note, that the formula for the amplitudes of scattered Floquet harmonics (47) contains series that have the same form as (50), but another sign in front of $k_{s,l}^x$.

The amplitudes of the excited modes A_i can be found numerically from the infinite set of equations (50) and substitution of A_i into (47) will give us amplitudes of scattered Floquet harmonics. However, it is possible to obtain a closed-form analytical solution of (50).

In order to solve the set of equations (50) one should consider a characteristic function $f(x)$ (see also [21]) of the form :

$$f(u) = u \sum_i A_i \frac{1}{u - e^{jq_x^{(i)} a}}. \quad (51)$$

Comparing (47) and (50) with (51) one can see that the function $f(u)$ has the following properties:

- It has poles at $u = e^{jq_x^{(i)} a}$
- It has roots at $u = e^{jk_{s,l}^x a}$, $(s,l) \neq (0,0)$ and $u = 0$
- It has a known value $E_{\text{inc}}/\gamma_{0,0}^{+}$ at $u = e^{jk_x a}$
- Its values at $u = e^{-jk_{s,l}^x a}$ are equal to the normalized amplitudes of scattered Floquet harmonics
- Its residues at $u = e^{jq_x^{(i)} a}$ are equal to the normalized amplitudes of excited eigenmodes.

It is possible to restore the function $f(u)$ using the known values of its poles, roots and a value at one point:

$$f(u) = \frac{E_{\text{inc}} u}{\gamma_{0,0}^{+} e^{jk_x a}} \prod_{(s,l)\neq(0,0)} \frac{u - e^{jk_{s,l}^x a}}{e^{jk_x a} - e^{jk_{s,l}^x a}} \prod_i \frac{e^{jk_x a} - e^{jq_x^{(i)} a}}{u - e^{jq_x^{(i)} a}}. \quad (52)$$

The knowledge of the characteristic function $f(u)$ provide us with complete solution of our diffraction problem. The amplitudes of excited eigenmodes with indices n are equal to residues of $f(u)$ at $u = e^{jq_x^{(n)} a}$:

$$A_n = \text{Res} f(u) \Big|_{u=e^{jq_x^{(i)}a}} = \frac{E_{\text{inc}}(1 - e^{j(q_x^{(n)} - k_x)a})}{\gamma_{0,0}^{+}} \times$$

$$\times \prod_{(s,l)\neq(0,0)} \frac{e^{jq_x^{(n)} a} - e^{jk_{s,l}^x a}}{e^{jk_x a} - e^{jk_{s,l}^x a}} \prod_{i \neq n} \frac{e^{jk_x a} - e^{jq_x^{(i)} a}}{e^{jq_x^{(n)} a} - e^{jq_x^{(i)} a}}, \quad (53)$$

and the amplitudes of scattered Floquet harmonics with indices (r,t) can be expressed through values of $f(u)$ at $u = e^{-jk_{r,t}^x a}$:

$$\mathbf{E}_{r,t} = \frac{E_{\text{inc}} e^{-jk_{r,t}^x a} [\mathbf{k}_{r,t}^{-} \times [\mathbf{k}_{r,t}^{-} \times \mathbf{d}]]}{2jab\varepsilon_0 k_{r,t}^x \gamma_{0,0}^{+} e^{jk_x a}} \times$$

$$\times \prod_{(s,l)\neq(0,0)} \frac{e^{-jk^x_{r,t}a} - e^{jk^x_{s,l}a}}{e^{jk_x a} - e^{jk^x_{s,l}a}} \prod_i \frac{e^{jk_x a} - e^{jq^{(i)}_x a}}{e^{-jk^x_{r,t}a} - e^{jq^{(i)}_x a}}. \quad (54)$$

The products in the formulae (53) and (54) have very rapid convergence. It is enough to take a few terms in order to reach excellent accuracy. The main requirement for truncation of these infinite products is to take into account all terms corresponding to propagating $\mathrm{Re}(k^x_{s,l}) = 0$ and slowly decaying $\mathrm{Im}(k^x_{s,l}) \ll 2\pi/a$ Floquet harmonics as well as propagating $\mathrm{Re}(q^{(i)}_x) = 0$ and slowly decaying $\mathrm{Im}(q^{(i)}_x) \ll 2\pi/a$ eigenmodes.

F. Comparison with other theories

Let us consider the case from work [10] when $\mathbf{d} = \mathbf{y}_0$, and $a = b = c$. In this case the formula (54) for the fundamental Floquet harmonic ($r = t = 0$) can be rewritten in terms of the reflection coefficient:

$$R = -e^{-2jk_x a} \prod_{(s,l)\neq(0,0)} \frac{e^{-jk_x a} - e^{jk^x_{s,l}a}}{e^{jk_x a} - e^{jk^x_{s,l}a}} \prod_i \frac{e^{jk_x a} - e^{jq^{(i)}_x a}}{e^{-jk_x a} - e^{jq^{(i)}_x a}}. \quad (55)$$

Comparing that result with the final result of the work [10] (the next formula after (C7) on page 841) one can see that the first product in our formula (55)

$$\Pi = \prod_{(s,l)\neq(0,0)} \frac{e^{-jk_x a} - e^{jk^x_{s,l}a}}{e^{jk_x a} - e^{jk^x_{s,l}a}} \quad (56)$$

is absent in the result of Mahan and Obermair. This difference is a consequence of the fact that in our study we considered interaction between crystal planes accurately taking into account all Floquet harmonics for any distance between planes in contrast to the "near-neighbor approximation" used in the approach of Mahan and Obermair.

The dependence of the product Π vs. normalized frequency is plotted in Figure 7 for the case of normal incidence $k_y = k_z = 0$ and $k_x = k$. One can see that the value of the product is nearly equal to the unity for $ka < 1.6\pi$, but for $ka > 2\pi$ the value of the product significantly differs from the unity. Thus we conclude that the theory of Mahan and Obermair is valid in the low frequency range when periods of the lattice are small compared to the wavelength. Our theory does not have such a restriction (within the frame of the dipole model of electromagnetic crystal).

The comparison with results of [21] shows that (55) is equivalent to formula (46) from [21] with $\Pi = \exp(\Gamma)$ where Γ is given by the contour integral (47) from [21]. The calculation of Π using (56) requires taking into account only a few terms in the infinite products, because they are very rapidly convergent. This is a significant advantage of our approach as compared to work [21] which requires complicate numerical calculation of the contour integral.

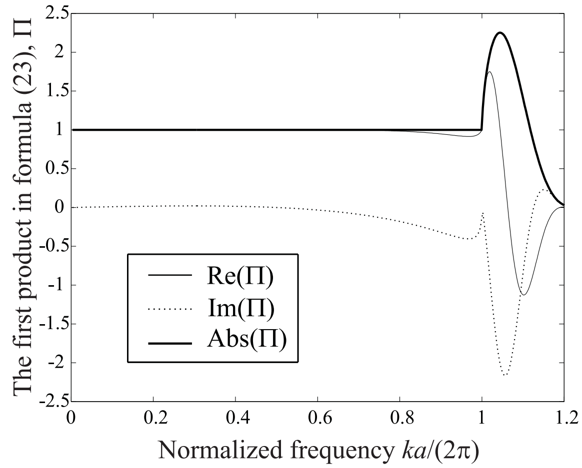

FIG. 7: Dependence of Π vs. normalized frequency $ka/(2\pi)$

In the long-wavelength limit, the series in equation (34) for the cubic lattice can be replaced by the integral taken over the whole space except unit cell V and we obtain:

$$\alpha^{-1} = \left[\left(\int_{R^3/V} \overline{\overline{G}}(\mathbf{R}) e^{-j(\mathbf{q}\cdot\mathbf{R})} d\mathbf{R}\right)\mathbf{d}\right]\cdot\mathbf{d}. \quad (57)$$

The integral in the right-hand side of equation (57) can be evaluated by means of the same technique that was used while deducing Ewald-Oseen extinction principle in [9]. The result is following:

$$\alpha^{-1} = \left[\frac{1}{3} + \frac{(\mathbf{q}\cdot\mathbf{d})^2 - |\mathbf{q}|^2}{K^2 - |\mathbf{q}|^2}\right]\frac{V}{\varepsilon_0}. \quad (58)$$

The obtained dispersion equation (58) can be transformed in the common form:

$$\tilde{\varepsilon}(k^2 - q_d^2) = \varepsilon_0(|\mathbf{q}|^2 - q_d^2), \quad (59)$$

where

$$\tilde{\varepsilon} = \varepsilon_0\left(1 + \frac{\alpha/(\varepsilon_0 V)}{1 - \alpha/(3\varepsilon_0 V)}\right), \quad (60)$$

and $q_d = (\mathbf{q}\cdot\mathbf{d})$ is the component of the wave vector $\mathbf{q}$ along the anisotropy axis.

The formula (59) is classical form of the dispersion equation for uniaxial dielectrics [9] with permittivity $\tilde{\varepsilon}$ along the anisotropy axis and ε in the transverse plane. The expression (60) is the Clausius-Mossotti formula for the effective permittivity of cubic lattices of scatterers.

In the long-wavelength limit the formula (54) for amplitude of reflected wave simplifies as follows:

$$\mathbf{E}_R = -\frac{(\mathbf{E}_{\rm inc}\cdot\mathbf{d})[\mathbf{k}^-\times[\mathbf{k}^-\times\mathbf{d}]]}{[k^2 - (\mathbf{k}\cdot\mathbf{d})^2]}\frac{k_x - q_x}{k_x + q_x}, \quad (61)$$

where $\mathbf{k}^- = (-k_x, k_y, k_z)^T$ is wave vector of reflected wave. The formula (61) represents a compact form of an expression for electric field amplitude of a wave reflected from an interface between an isotropic dielectric and an uniaxial dielectric (see, e.g. [30]). Note, that in our case the situation is simplified as compared to the general case, because the incident wave comes from isotropic dielectric with permittivity ε which is equal to the permittivity of uniaxial dielectric in transverse plane. It means, that an incident wave with normal polarization with respect to the anisotropy axis transforms at the interface in a refracted ordinary wave without reflection.

Let us consider the reflection problem at the special case when $\mathbf{d} = \mathbf{y}_0$, $k_y = 0$ and $\mathbf{E}_{\rm inc} \parallel \mathbf{y}_0$. The nonzero components of the wave vector for the incident wave can be expressed in terms of incident angle θ_i as $k_z = k\sin\theta_i$ and $k_x = k\cos\theta_i$. From (59) we obtain that in this case the transmitted wave has x-component of wave vector equal to $q_x = \sqrt{\tilde{\varepsilon}k^2/\varepsilon_0 - k_z^2} = \sqrt{\tilde{\varepsilon}/\varepsilon_0}k\cos\theta_t$, where θ_t in angle or refraction. With the result (61) we get the reflection coefficient in the form:

$$R = \frac{k_x - q_x}{k_x + q_x} = \frac{n_1\cos\theta_i - n_2\cos\theta_t}{n_1\cos\theta_i + n_2\cos\theta_t}, \tag{62}$$

where $n_1 = \sqrt{\varepsilon_0\mu_0}$ and $n_2 = \sqrt{\tilde{\varepsilon}\mu_0}$ are indices of refraction of the materials. The formula (62) coincide with the classical Fresnel equation [9]. This fact can be treated as an additional verification of presented theory.

IV. LATTICE OF SPLIT-RING-RESONATORS

In this section we apply theory presented in previous sections for study of reflection from semi-infinite cubic lattice of split-ring-resonators.

The general dispersion equation (6) of the integral form in the case of point electric scatterers transforms into transcendental equation (38). In the case when $\mathbf{d} = \mathbf{y}_0$ the dispersion equation (38) can be rewritten in the following closed form convenient for numerical calculations (see [11] for details):

$$\varepsilon_0\alpha^{-1}(\omega) = C(k, \mathbf{q}, a, b, c), \tag{63}$$

where $C(k, \mathbf{q}, a, b, c)$ is dynamic interaction constant of the form:

$$C(k,\mathbf{q},a,b,c) = -\sum_{l=1}^{+\infty}\sum_{\mathrm{Re}(p_s)\neq 0}\frac{p_s^2}{\pi b}K_0\left(p_s c l\right)\cos(q_z c n)$$

$$+\sum_{s=-\infty}^{+\infty}\sum_{l=-\infty}^{+\infty}\frac{p_s^2}{2jbck_{s,l}^x}\frac{e^{-jk_{s,l}^x a} - \cos q_x a}{\cos k_{s,l}^x a - \cos q_x a} \tag{64}$$

$$-\sum_{\mathrm{Re}(p_s)=0}\frac{p_s^2}{2bc}\left(\frac{1}{jk_{s,0}^x} + \sum_{l=1}^{+\infty}\left[\frac{1}{jk_{s,l}^x} + \frac{1}{jk_{s,-l}^x}\right.\right.$$

$$\left.\left. -\frac{c}{\pi l} - \frac{r_s c^3}{8\pi^3 l^3}\right] + 1.202\frac{r_s c^3}{8\pi^3} + \frac{c}{\pi}\left(\log\frac{c|p_s|}{4\pi} + \gamma\right) + j\frac{c}{2}\right)$$

$$+\frac{1}{4\pi b^3}\left[4\sum_{s=1}^{+\infty}\frac{(2jkb+3)s+2}{s^3(s+1)(s+2)}e^{-jkbs}\cos(q_y bs)\right.$$

$$-(jkb+1)\left(t_+^2\log t^+ + t_-^2\log t^- + 2e^{jkb}\cos(q_y b)\right)$$

$$\left.-2jkb\left(t_+\log t^+ + t_-\log t^-\right) + (7jkb+3)\right],$$

and the following notations are used:

$$p_s = \sqrt{(k_s^y)^2 - k^2}, \qquad r_s = 2q_z^2 - p_s^2,$$

$$t^+ = 1 - e^{-j(k+q_z)c}, \qquad t^- = 1 - e^{-j(k-q_z)c},$$

$$t_+ = 1 - e^{j(k+q_z)c}, \qquad t_- = 1 - e^{j(k-q_z)c}.$$

The calculations using (64) can be restricted to the real part of dynamic interaction constant $C(k, \mathbf{q}, a, b, c)$ only, because its imaginary part is given by much simpler expression (see [11] for details):

$$\mathrm{Im}\left\{C(k,\mathbf{q},a,b,c)\right\} = \frac{k^3}{6\pi}. \tag{65}$$

The series in (64) have excellent convergence that ensure very rapid numerical calculations.

The case of magnetic scatterers can be considered using duality principle. The expression (55) can be used for calculation of reflection coefficient by magnetic field (originally, this equation represented reflection coefficient by electric field). The dispersion equation (63) have to be rewritten for the case of magnetic point scatterers in the following form:

$$\mu_0\alpha_m^{-1}(\omega) = C(k, \mathbf{q}, a, b, c), \tag{66}$$

where $\alpha_m(\omega)$ is magnetic polarizability of the scatterers. The analytical expressions for the magnetic polarizability $\alpha(\omega)$ of split-ring-resonators with geometry plotted in Fig.4 were derived and validated in [31]. The final result reads as follows [11]:

$$\alpha(\omega) = \frac{A\omega^2}{\omega_0^2 - \omega^2 + j\omega\Gamma}, \tag{67}$$

where A is amplitude, ω_0 is resonant frequency and $\Gamma = A\omega k^3/(6\pi\mu_0)$ is the radiation reaction factor. The expressions for amplitude A and resonant frequency ω_0 in terms of dimensions of split-ring-resonators are available in [11, 31]. In the present paper we will use typical parameters $A = 0.1\mu_0 a^3$ and $\omega_0 = 1/(a\sqrt{\varepsilon_0\mu_0})$.

The dispersion properties of cubic lattice of split-ring-resonators with such parameters have been extensively studied in [11]. Using the theory of the present paper we will study reflection properties of such a metamaterial. Let us consider the case of cubic lattice ($a = b = c$), normal incidence ($k_y = k_z = 0$) and let the magnetic field of incident wave is along directions of magnetic dipoles $\mathbf{d} = \mathbf{y}_0$. Numerical solution of dispersion equation (66) with $q_y = k_y = 0$ and $q_z = k_z = 0$ allows to get a set of wave vectors of excited eigenmodes $\{q_i^x\}$. These wave vectors are plotted at the top of Fig. 8 as functions of normalized frequency ka. The point $ka = 1$ corresponds to the resonant frequency ω_0 os split-ring-resonators. One can see that the propagating modes ($\mathrm{Im}(q_x) = 0$) exist only for $ka \leq 0.978$ and $ka \geq 1.044$. It means that a partial resonant band gap is observed for $ka \in [0.978, 1.044]$. At the frequencies inside of the band gap all the eigenmodes decay with distance. Note, that such decaying modes exist at all frequencies, not only inside of the band gap. The Fig. 8 shows only the eigenmodes with slowest decay $|\mathrm{Im}(q_x)| < 1.5\pi/a$. There is an infinite number of other decaying modes which decay with distance more rapidly. The contribution of such modes into the reflection coefficient is negligible as it was shown above. The decaying modes can be separated into the three classes:

- evanescent modes, the modes which have $\mathrm{Re}(q_x) = 0$, they decay exponentially from one crystal plane to the other one;
- staggered modes, the modes which have $\mathrm{Re}(q_x) = \pi/a$, they exponentially decay from one crystal plane to the other one by absolute value, but the dipoles in the neighboring plane are excited in out of phase;
- complex modes, the most general case of the decaying modes which have $\mathrm{Re}(q_x) \neq 0$, they experience both exponential decay and phase variation from one crystal plane to the other one.

The evanescent modes are the most common type of decaying modes. They can be observed in dielectrics with negative permittivity, for example. The staggered modes are limiting case of the complex modes and can be widely observed in periodical structures in vicinity of the band gap edges, see for example [32, 33]. The complex modes of general kind are quite exotic for common materials.

In the system under consideration we are able to observe all three kind of mentioned decaying modes. The presence of staggered and complex modes are evidence of spatial dispersion in this material reported in [11]. The staggered modes exists for $ka \geq 0.984$, evanescent modes for $ka \geq 1.015$ and complex modes for $ka \in [0.984, 1.015]$ (see Fig. 8). One can see that for a fixed frequency from the range $ka \in [0.978, 0.984]$ there are two staggered modes and in the range $ka \in [1.015, 1.044]$ there are two evanescent modes. Actually, in the range $ka \in [0.984, 1.015]$ there are also two complex modes which have the same imaginary parts but differs by sign of the real part. Thus, we conclude that for every frequency from the range $ka \in [0.95, 1.08]$ that we consider the incident wave will excite in the crystal a pair of modes with $|\mathrm{Im}(q_x)| < 1.5\pi/a$ (propagating and staggered, two staggered, two complex, two evanescent or propagating and evanescent). Using the usual approach one has to introduce an additional boundary condition to solve this problem since usual condition of tangential component continuity is not enough in the case of excitation of two modes.

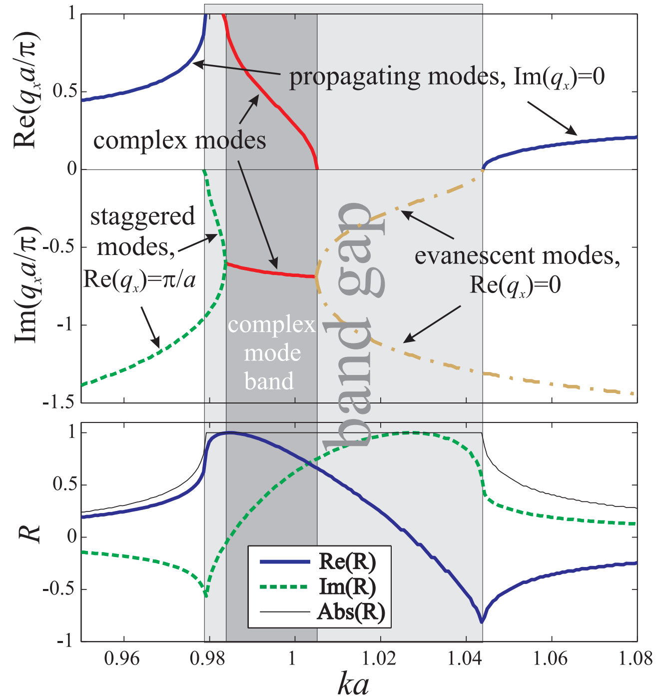

FIG. 8: (Color online) Dependencies of the normalized wave vectors $q_x a/\pi$ of excited eigenmodes (imaginary and real parts) and the reflection coefficient R calculated using (55) on normalized frequency ka for semi-infinite cubic lattice of split-ring-resonators with $A = 0.1\mu_0 a^3$ and $\omega_0 = 1/(a\sqrt{\varepsilon_0\mu_0})$.

Using the theory introduced in the previous section it is enough to substitute obtained wave vectors of eigenmodes into (55) the reflection coefficient is calculated. The reflection coefficient is plotted at the bottom of Fig. 8. One can see that at the frequencies in vicinity of the bottom and top edges of the band gap the semi-infinite crystal operate nearly as the electric and magnetic walls, respectively, as it was predicted in [32]. At the frequency $ka = 0.984$ the reflection coefficient is equal to $+1$ (electric wall), and at $ka = 1.044$ it is $-0.8 + 0.6j$ (nearly magnetic wall). Note, that the frequency corresponding to the electric wall effect is not equal to the bottom edge of the band gap and there are no frequency exactly corresponding to the magnetic wall effect. The use of the usual formulae for reflection coefficient from magnetic and Clausius-Mossotti formulae which do not take into account effects of spatial dispersion one could get idea that magnetic and magnetic wall effects have to

happen at the edges of the band gap. Our study demonstrate that if the spatial dispersion is taken into account accurately then it is not so.

Thus, we have demonstrated how the proposed theory can be used for modeling of reflection from semi-infinite crystals with spatial dispersion. Our theory can be treated as generalization of results of Mahan and Obermair [10] which have been widely applied for modeling of various kinds of reflection problems. We hope that the present generalization can find much more applications in modeling of reflection from spatially dispersive materials since in has no restriction on the period of the lattice to be smaller than wavelength and allows to consider electromagnetic crsytals of general kind.

V. CONCLUSION

In this paper a new approach for solving problems of plane-wave diffraction on semi-infinite electromagnetic crystals is proposed. The boundary conditions for the interface between isotropic dielectric and electromagnetic crystal of general kind are deduced in the form of infinite system of equations relating amplitudes of incident wave, excited eigenmodes and scattered spatial harmonics. This system of equations represent mathematical content of generalized Ewald-Oseen extinction principle which is formulated in this paper: the polarization of the semi-crystal excited by plane wave is distributed in such way that it cancels the incident wave together with all high-order spatial harmonics associated with periodicity of the boundary. In our opinion, the proof of generalized Ewald-Oseen extinction principle presented in this paper is an important theoretical fact which helps to understand interrelation between reflection and dispersion properties of electromagnetic crystals. If the eigenmodes of the infinite crystal are known then the system can be solved numerically which provides new numerical method for solving the diffraction problem under consideration. We believe in the quite good prospects for the application of the described method in further studies of dielectric and even metallic electromagnetic crystals at both microwave and optical ranges.

For the special case when the crystal is formed by small scatterers which can be effectively replaced by dipoles with fixed orientation the deduced system of equations is solved analytically using method of the characteristic function. The closed form expressions for the amplitudes of excited eigenmodes and scattered spatial harmonics are provided in terms of rapidly convergent products. These expressions can be treated as generalization of classical result of Mahan and Obermair [10] for the case when period of the lattice can be large as compared to the wavelength. The proposed method is applied for calculation of reflection coefficient from semi-infinite crystal formed by resonant magnetic scatterers (split-ring-resonators) at the frequencies corresponding to the strong spatial dispersion.

Acknowledgements

The authors would like to thank Sergei Tretyakov, Stanislav Maslovski and Mario Silveirinha for useful discussions of the material presented in this paper.

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